BENZYL CHLORIDE

Benzyl chloride is a federal hazardous air pollutant and was identified as a toxic air contaminant in April 1993 under AB 2728.

CAS Registry Number: 100-44-7

Molecular Formula: C₇H₇Cl



Benzyl chloride is a colorless to slightly yellow liquid with a pungent, aromatic odor. It is soluble in alcohol, ether, and chloroform, and is insoluble in water. It is very refractive. Benzyl chloride is combustible and is corrosive to metal. It reacts with steam and oxidizing agents and is slowly hydrolyzed by water (HSDB, 1991). Benzyl chloride also rapidly decomposes when heated in the presence of iron (Merck, 1989).

Physical Properties of Benzyl Chloride

Synonyms: alpha-chlorotoluene; omega-chlorotoluene; chloromethylbenzene; tolyl chloride; chlorophenylmethane

Molecular Weight:

Boiling Point:

Melting Point:

Flash Point:

126.58

179 °C

-48 to -43 °C

67.2 °C (153 °F)

Vapor Density: 4.4 (air = 1) Vapor Pressure: 1 mm Hg at 22 °C

Density/Specific Gravity: 1.10 at 20/20 °C (water=1)

Log Octanol/Water Partition Coefficient: 2.30

Conversion Factor: $1 \text{ ppm} = 5.18 \text{ mg/m}^3$

(HSDB, 1991; Merck, 1989; Sax, 1987; Sax, 1989; U.S. EPA, 1994a)

SOURCES AND EMISSIONS

A. Sources

Benzyl chloride is used in the manufacture of benzyl compounds, perfumes, pharmaceutical products, dyes, synthetic tannins, artificial resins, photographic developer, gasoline gum inhibitors, penicillin precursors, and quaternary ammonium compounds (HSDB, 1991).

The primary stationary sources that have reported emissions of benzyl chloride in California

Toxic Air Contaminant Identification List Summaries - ARB/SSD/SES September 1997 are sanitary services, chemical and allied products manufacturing, and educational services (ARB, 1997b).

B. Emissions

The total emissions of benzyl chloride from stationary sources in California are estimated to be at least 480 pounds per year, based on data reported under the Air Toxics "Hot Spots" Program (AB 2588) (ARB, 1997b).

C. Natural Occurrence

Benzyl chloride has not been reported as occurring in nature (HSDB, 1991).

AMBIENT CONCENTRATIONS

No Air Resources Board (ARB) data exist for ambient measurements of benzyl chloride.

INDOOR SOURCES AND CONCENTRATIONS

In an ARB study, benzyl chloride was not found in any indoor, outdoor, or personal air measurements except for one home. The mean indoor concentration of benzyl chloride was 0.85 micrograms per cubic meter (μ g/m³) (Sheldon et al, 1992).

ATMOSPHERIC PERSISTENCE

The dominant atmospheric loss process of benzyl chloride is expected to be by reaction with the hydroxy radical. The calculated half-life of benzyl chloride, due to its reaction with hydroxyl radicals, is estimated to be 3.5 days (Atkinson, 1989). The products of the hydroxyl radical reaction include Cloride atoms and benzaldehyde in low yield; other as yet unidentified products are formed (Tuazon et al, 1990).

AB 2588 RISK ASSESSMENT INFORMATION

The Office of Environmental Health Hazard Assessment reviews risk assessments submitted under the Air Toxics "Hot Spots" Program (AB 2588). Of the risk assessments reviewed as of April 1996, benzyl chloride did not contribute to the total cancer risk in any of the risk assessments reporting a total cancer risk equal to or greater than 1 in 1 million (OEHHA 1996a).

For non-cancer health effects, benzyl chloride did not contribute to the total hazard index in any of the risk assessments reporting a total chronic or acute hazard index greater than 1 (OEHHA, 1995).

HEALTH EFFECTS

Probable routes of human exposure to benzyl chloride are inhalation, ingestion, and dermal contact (U.S. EPA, 1994a).

Non-Cancer: Exposure to benzyl chloride may cause central nervous system depression, and irritation of the skin, eyes, nose, throat, and respiratory tract. High level exposure may cause pulmonary edema. Eye contact may result in immediate and severe eye irritation and prolonged exposure may cause permanent eye damage (Sittig, 1991; U.S. EPA, 1994a).

An acute non-cancer Reference Exposure Level (REL) of $50 \mu g/m^3$ and a chronic REL of $12 \mu g/m^3$ is listed for benzyl chloride in the California Air Pollution Control Officers Association Air Toxics "Hot Spots" Program, Revised 1992 Risk Assessment Guidelines. The toxicological endpoint considered for these values is the respiratory system (CAPCOA, 1993). The United States Environmental Protection Agency (U.S. EPA) has determined that the health effects data are inadequate for establishing a Reference Concentration (RfC) for benzyl chloride. The U.S. EPA has not established a Reference Dose (RfD) for benzyl chloride (U.S. EPA, 1994a).

No information is available on adverse reproductive or developmental effects of benzyl chloride in humans. One study has reported that rats orally exposed to benzyl chloride showed increases in embryonal mortality along with retarded development of the offspring (U.S. EPA, 1994a).

Cancer: Animal data indicate that long-term exposure to benzyl chloride by gavage increased the incidence of benign and malignant tumors at multiple sites and resulted in a significant increase in thyroid tumors in female rats (U.S. EPA, 1994a).

The U.S. EPA has classified benzyl chloride as Group B2: Probable human carcinogen with an oral unit risk estimate of 4.9 x 10⁻⁶ (microgram per liter)⁻¹. The U.S. EPA estimates that, if an individual were to ingest water containing benzyl chloride at 0.2 microgram per liter over his or her entire lifetime, that person would theoretically have no more than a 1 in 1 million increased chance of developing cancer (U.S. EPA, 1994a). The International Agency for Research on Cancer has not classified benzyl chloride for carcinogenicity (IARC, 1987a).

The State of California has determined under Proposition 65 that benzyl chloride is a carcinogen (CCR, 1996). The inhalation potency factor that has been used as a basis for regulatory action in California is 4.9×10^{-5} (microgram per cubic meter)⁻¹ (OEHHA, 1994). In other words, the potential excess cancer risk for a person exposed over a lifetime to $1 \mu g/m^3$ of benzyl chloride is estimated to be no greater than 49 in 1 million. The oral potency factor that has been used as a basis for regulatory action in California is 1.7×10^{-1} (milligram per kilogram per day)⁻¹ (OEHHA, 1994).